

4-Nitrosodiphenylamine
156-10-5 | DTXSID1021031

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 10.3

Global applicability domain: Inside

Local applicability domain index: 4.26e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

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Benzothiazole

Measured: 7.59

Predicted: 6.05

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N,N-Diethylaniline

Measured: 102

Predicted: 12.8

[Image not found](#)

N-Ethylaniline

Measured: 12.9

Predicted: 5.70

[Image not found](#)

Isophorone

Measured: 2.00

Predicted: 3.19